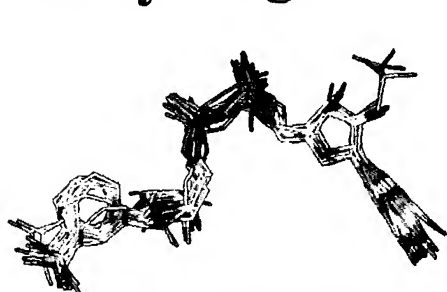
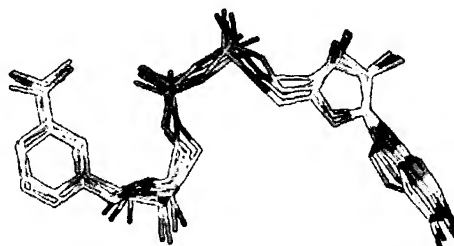


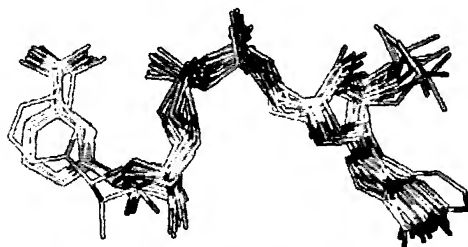
# Dehydrogenase Pharmacoclusters



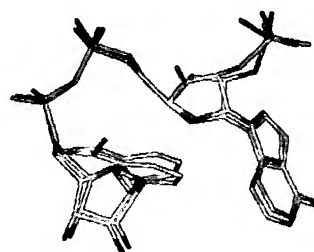
**Pharmacocluster 1**



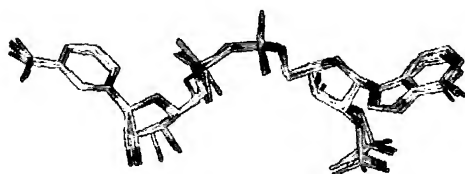
**Pharmacocluster 2**



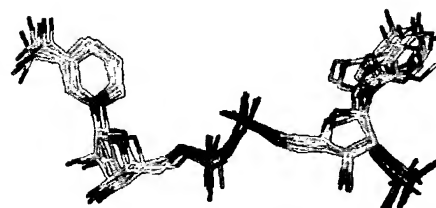
**Pharmacocluster 3**



**Pharmacocluster 4**



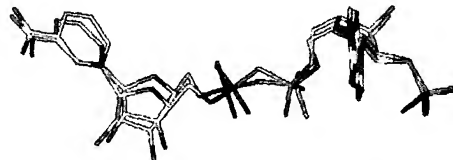
**Pharmacocluster 5**



**Pharmacocluster 6**



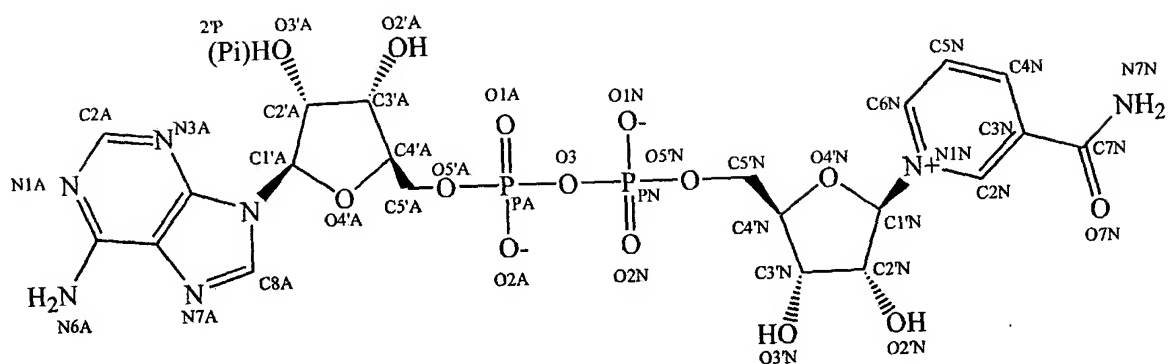
**Pharmacocluster 7**

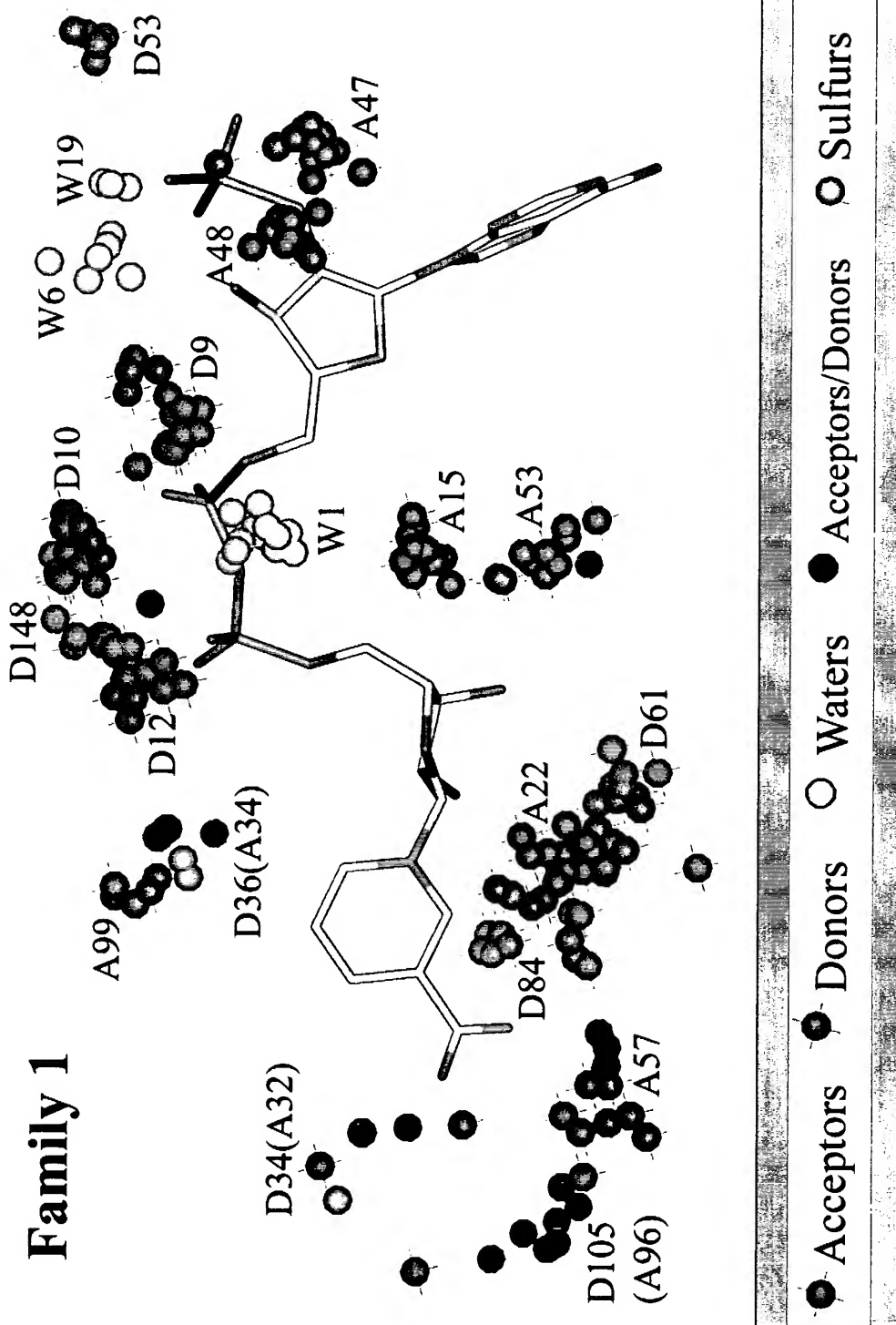


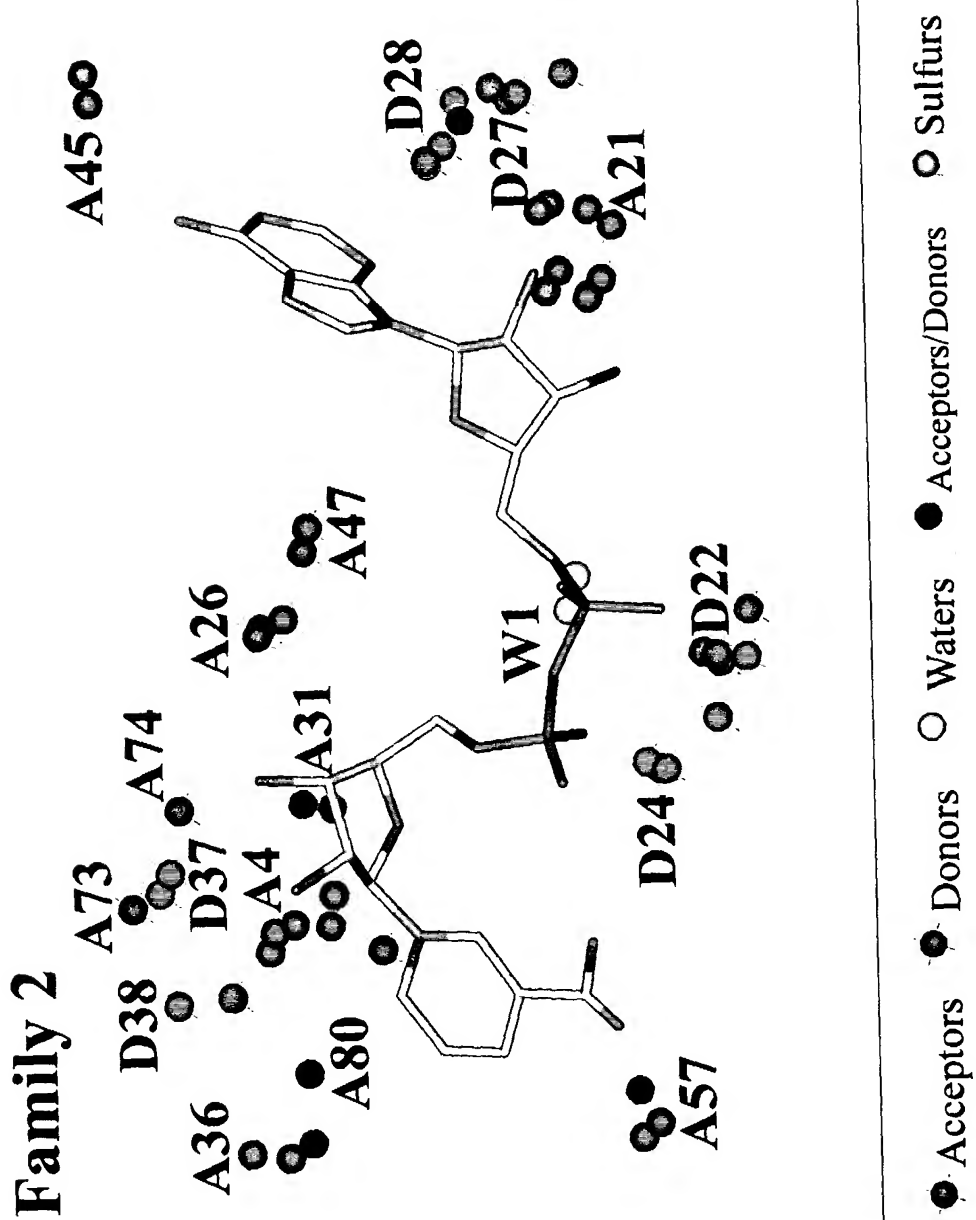
**Pharmacocluster 8**

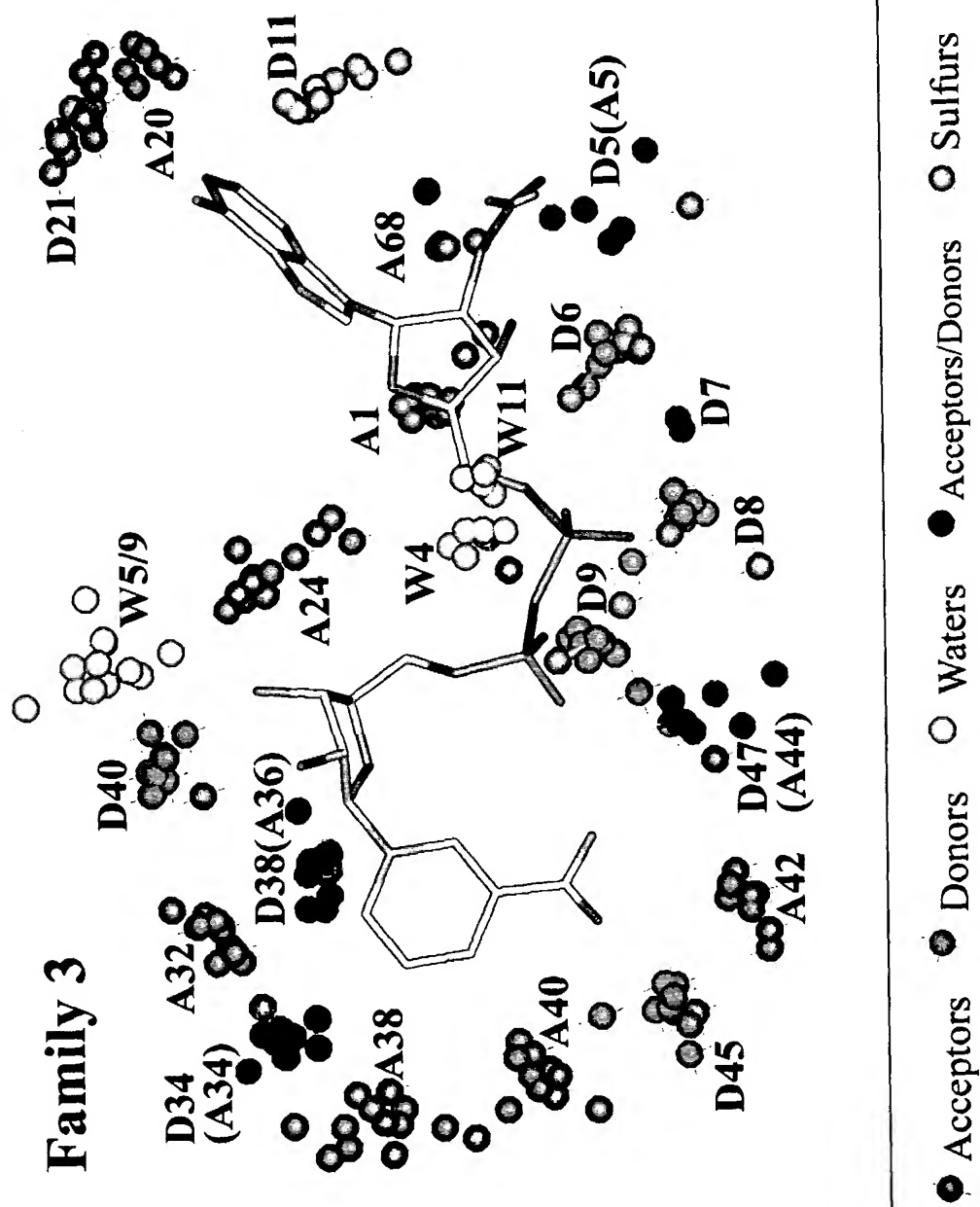
1004095.12001

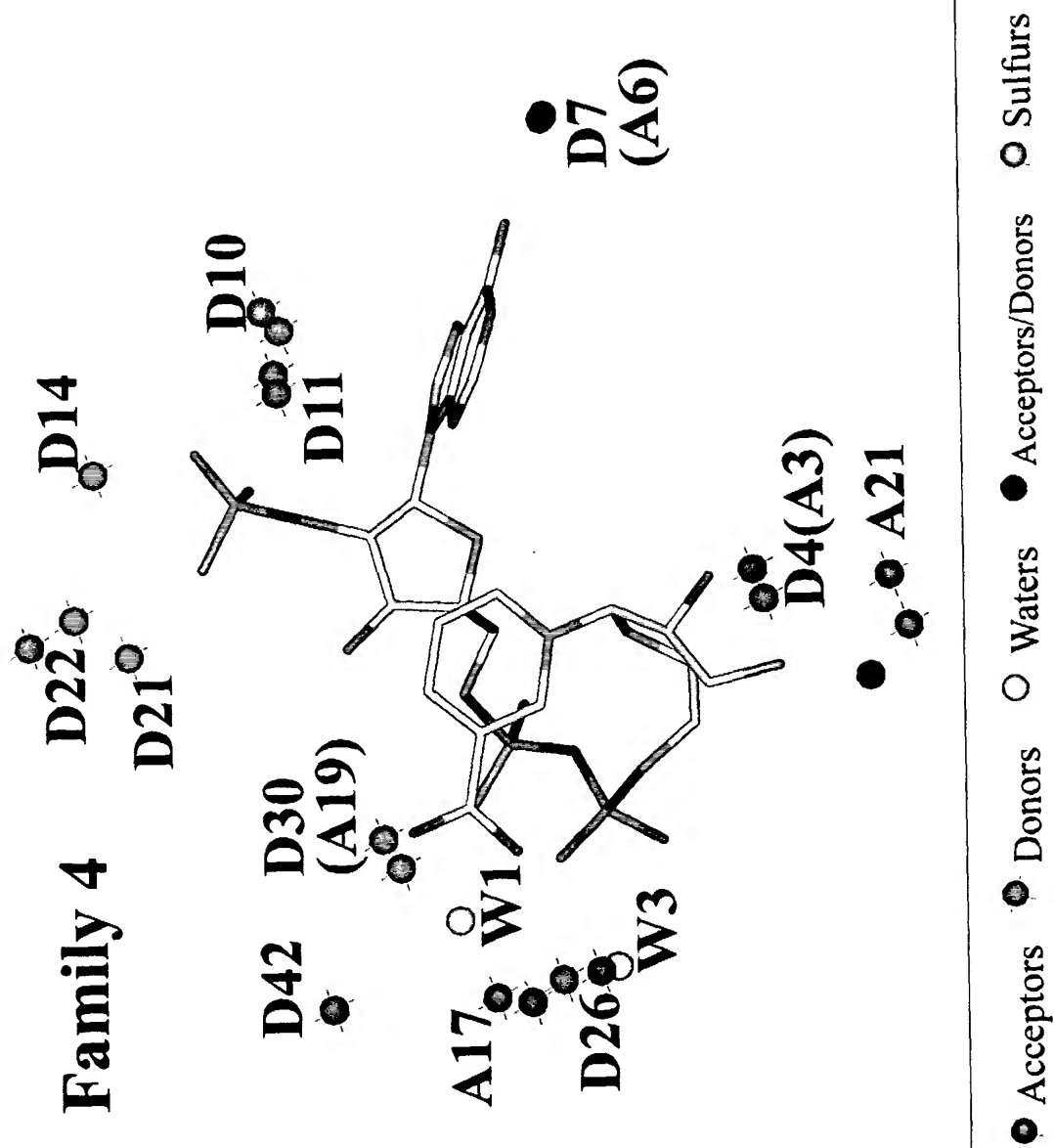
Figure 1 is a schematic representation of the experimental design. It shows a vertical timeline of events for two groups: 'Control' and 'Experimental'. The timeline starts with 'Baseline' and ends with 'Post-test'. Key events include 'Pre-test', 'Training', 'Post-training', 'Post-test', and 'Follow-up'. The 'Control' group receives 'Training' and 'Post-training' interventions, while the 'Experimental' group receives 'Training' and 'Post-training' interventions. The 'Control' group also receives 'Post-test' and 'Follow-up' interventions. The 'Experimental' group receives 'Post-test' and 'Follow-up' interventions. The timeline is divided into 'Pre-test', 'Training', 'Post-training', 'Post-test', and 'Follow-up' phases.

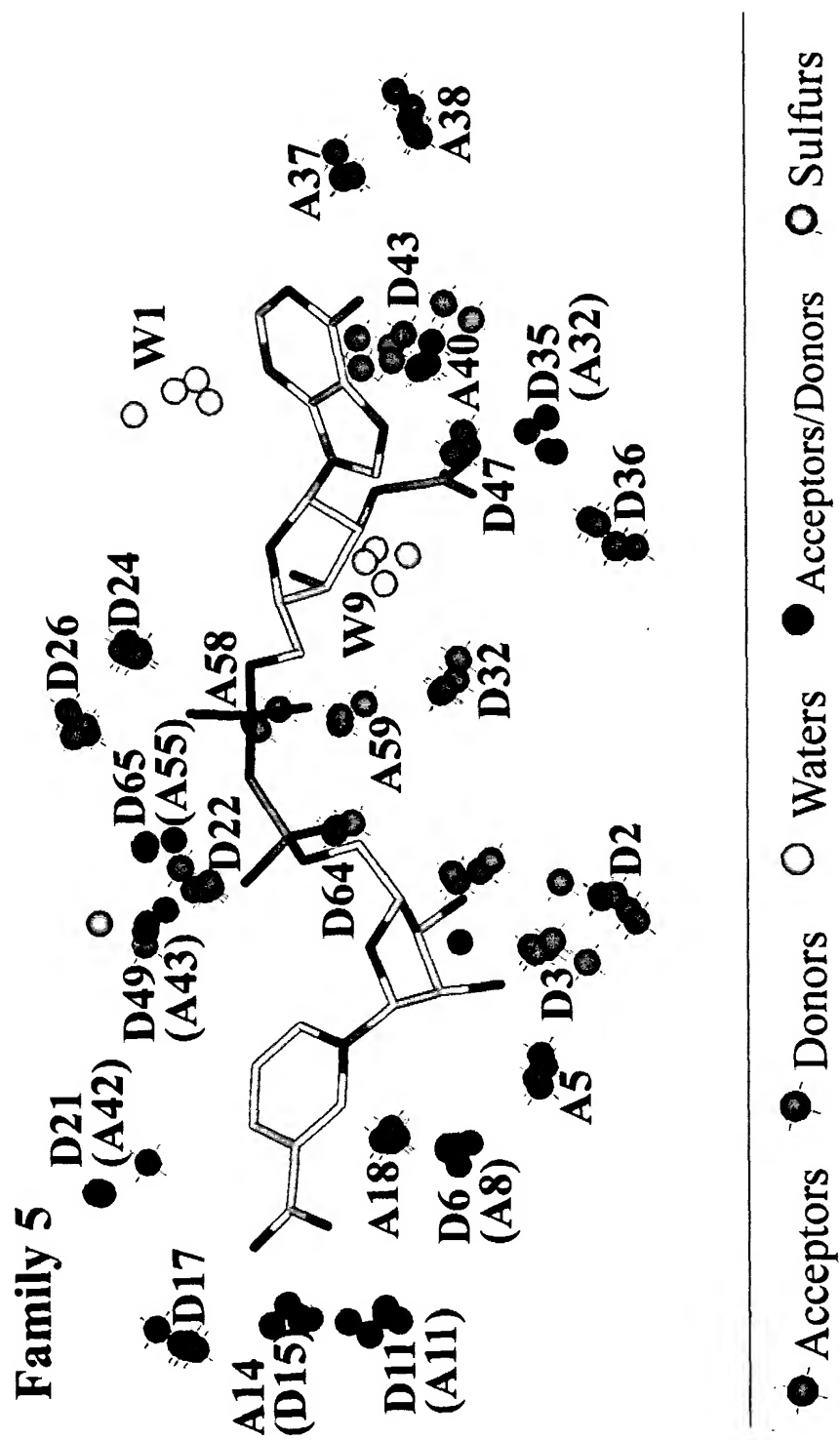


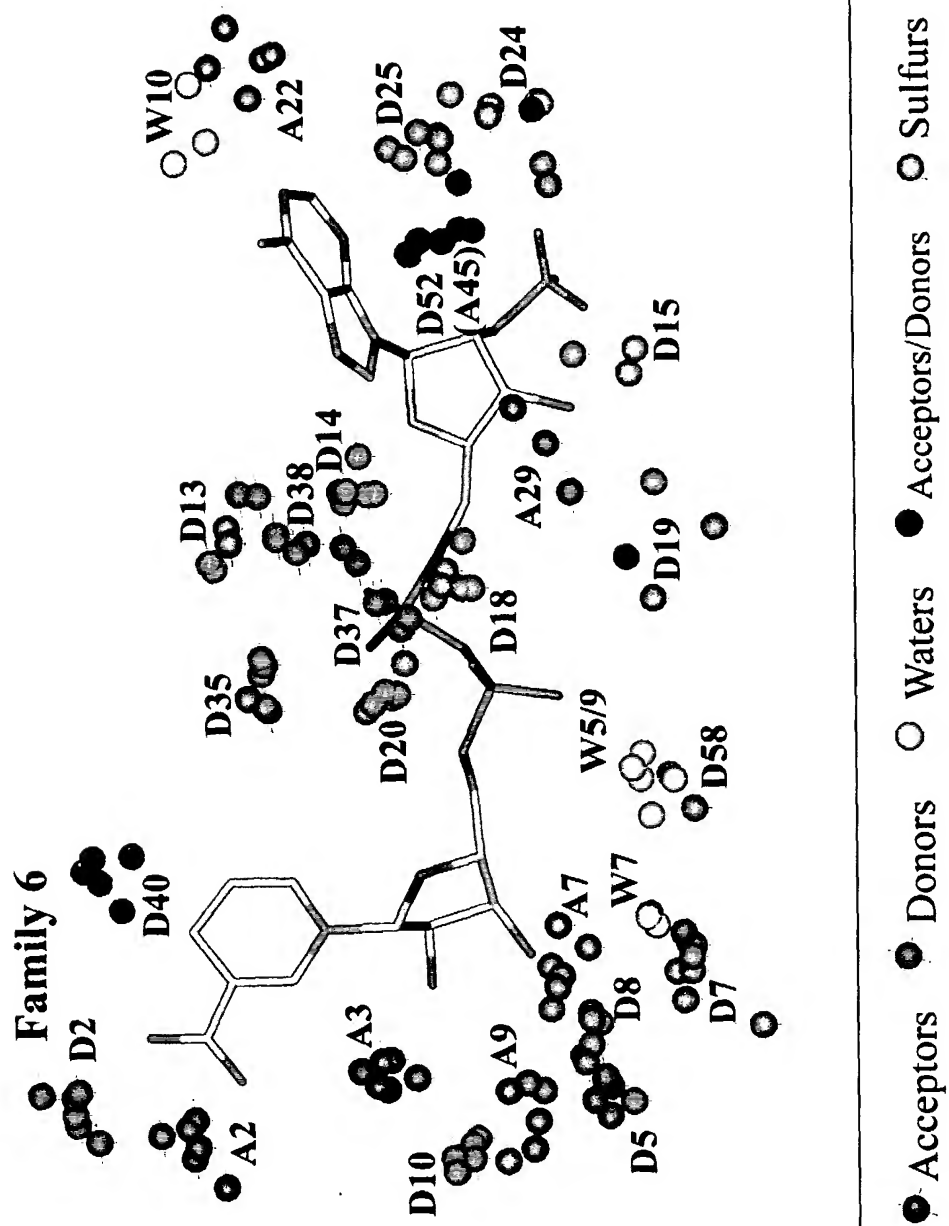




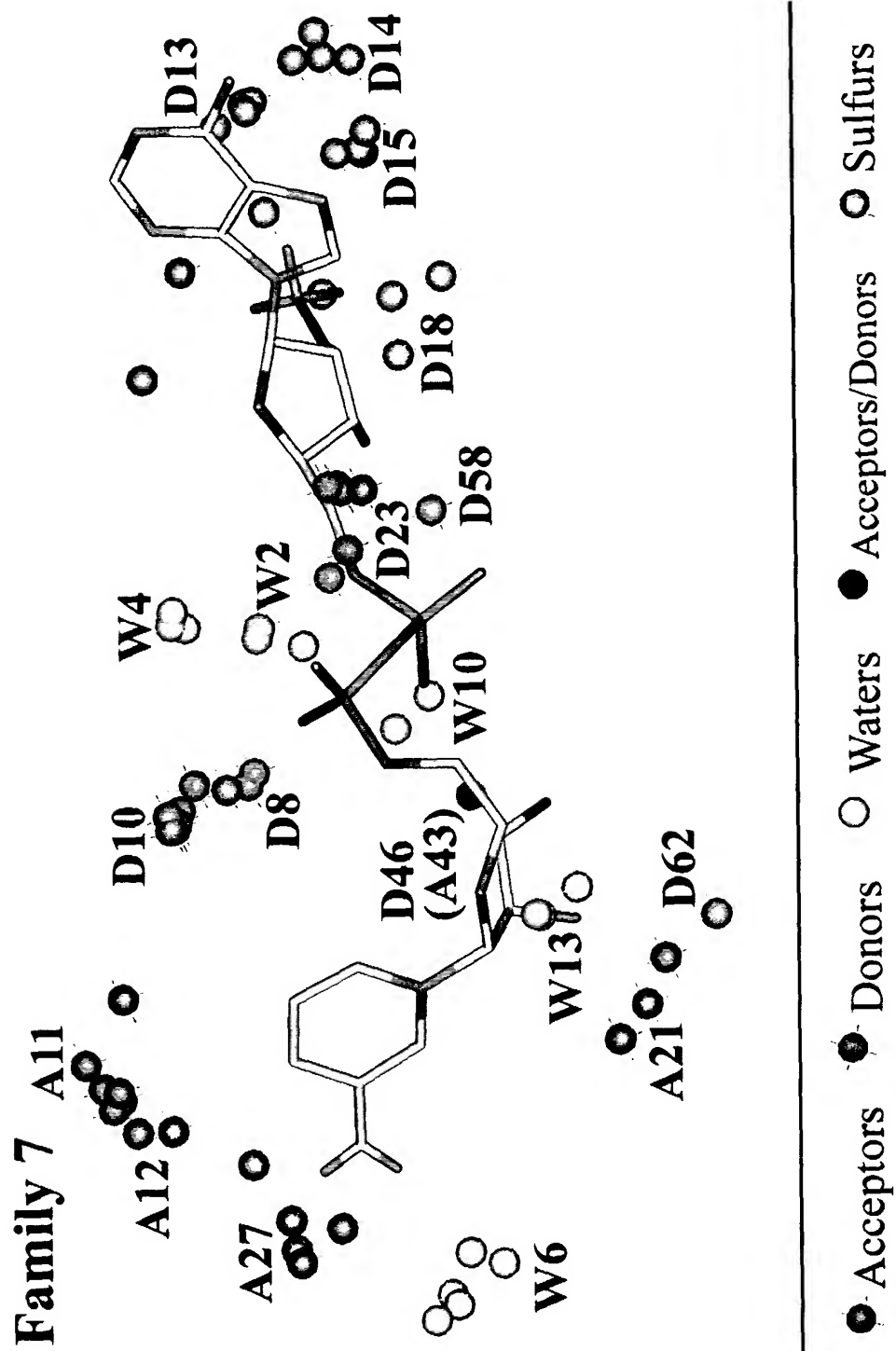


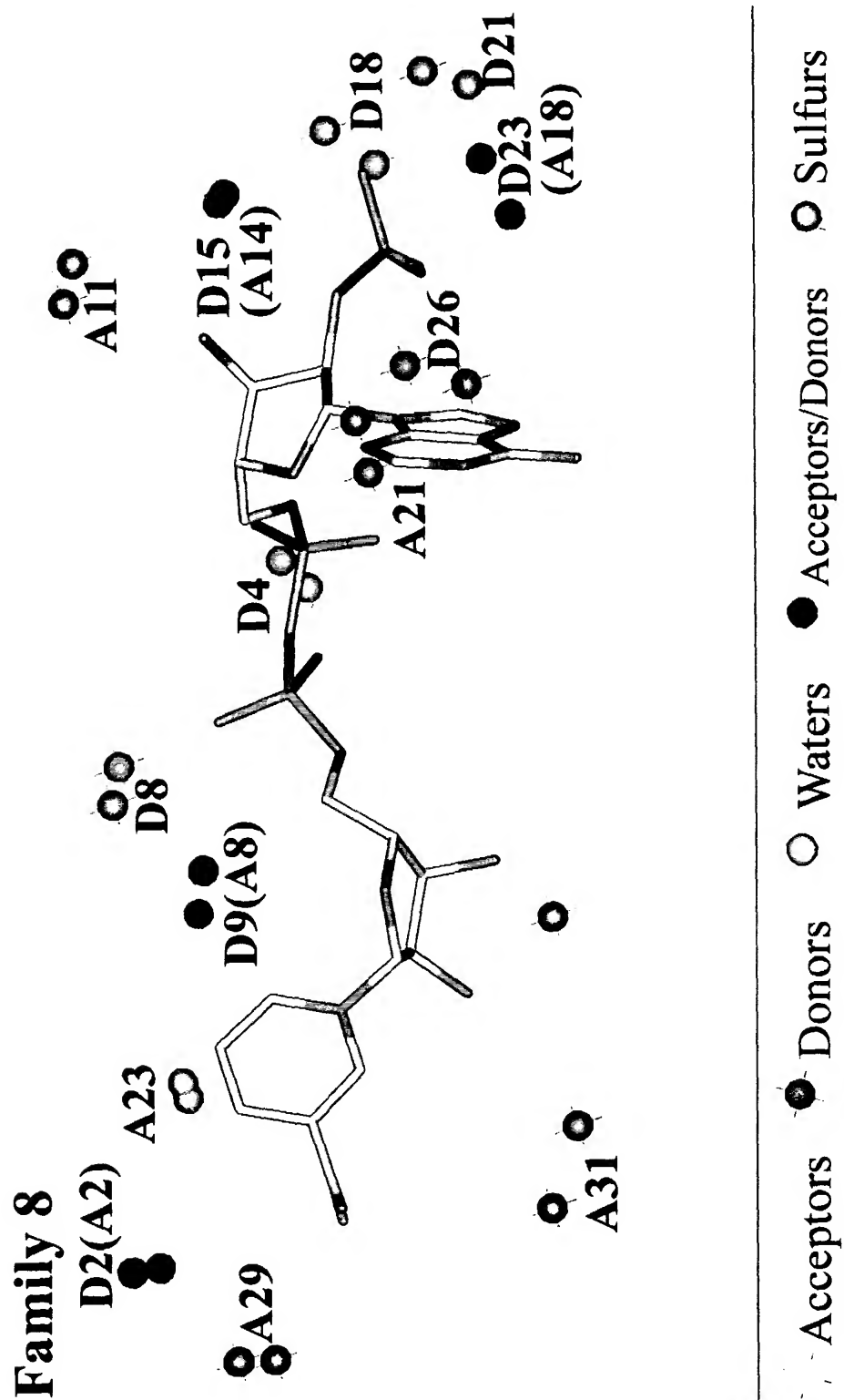


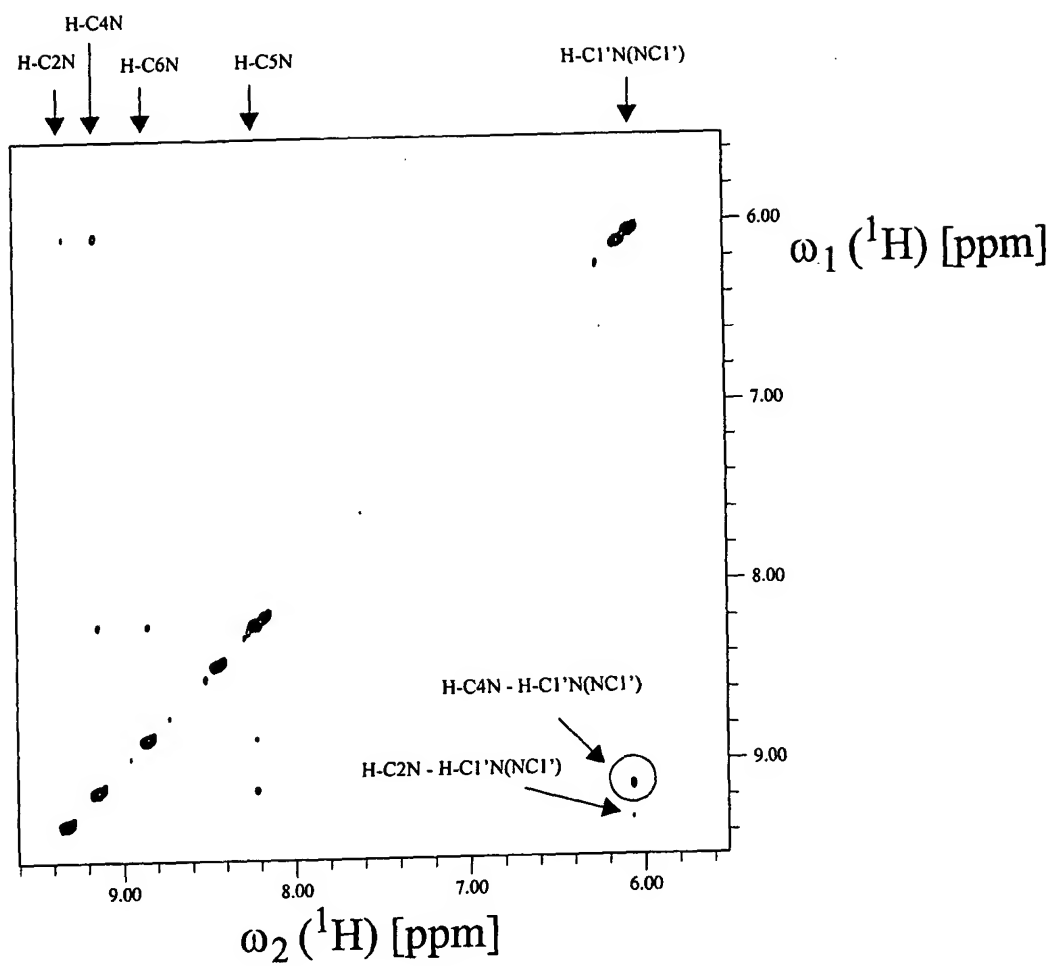






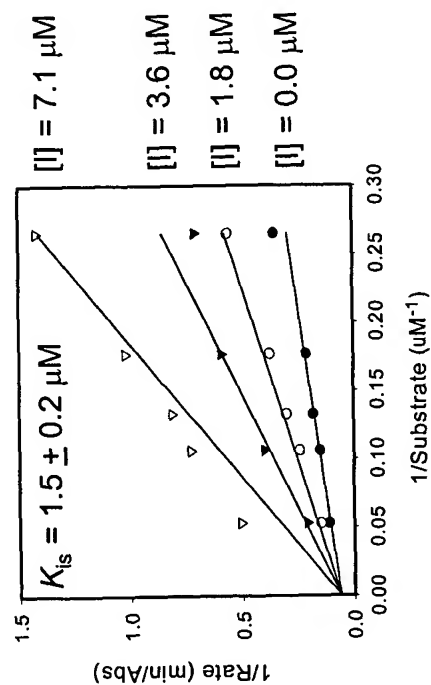




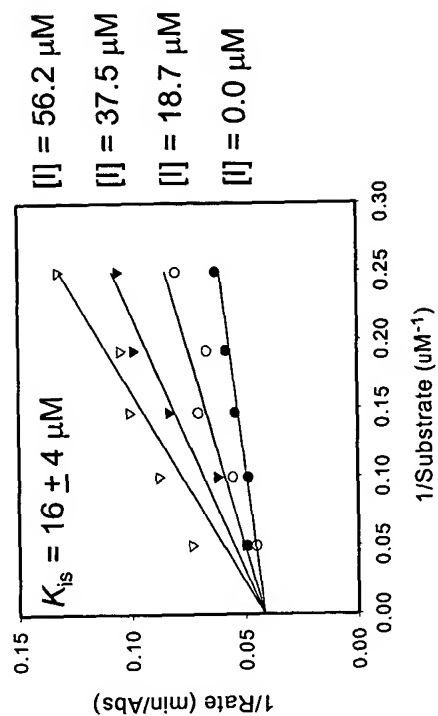


1009900000

**A.**  
Compound: TTE0001.001.A7  
Pharmacofamily 1 exemplar



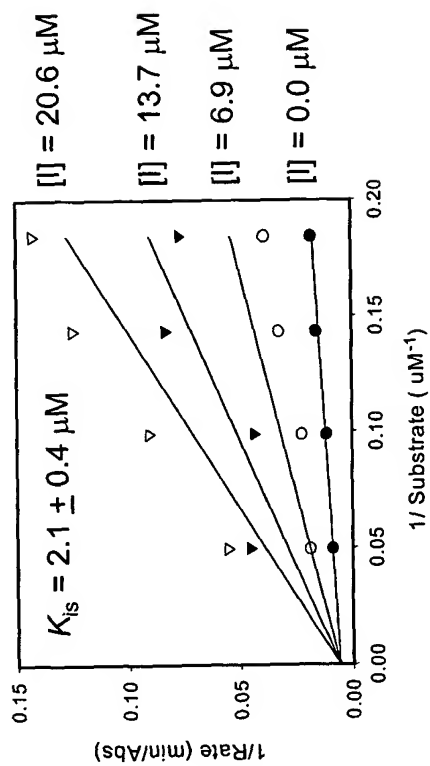
**B.**  
Compound: TTE0001.001.A7  
Pharmacofamily 8 exemplar



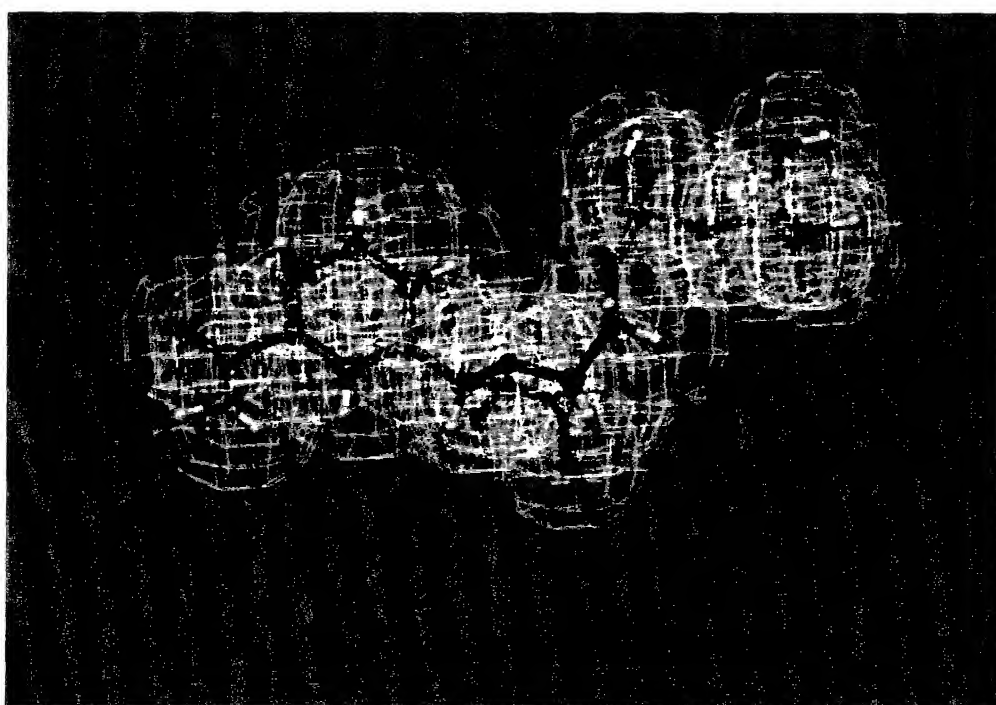
**B.**  
Compound: TTE0001.002.D2  
Pharmacofamily 8 exemplar

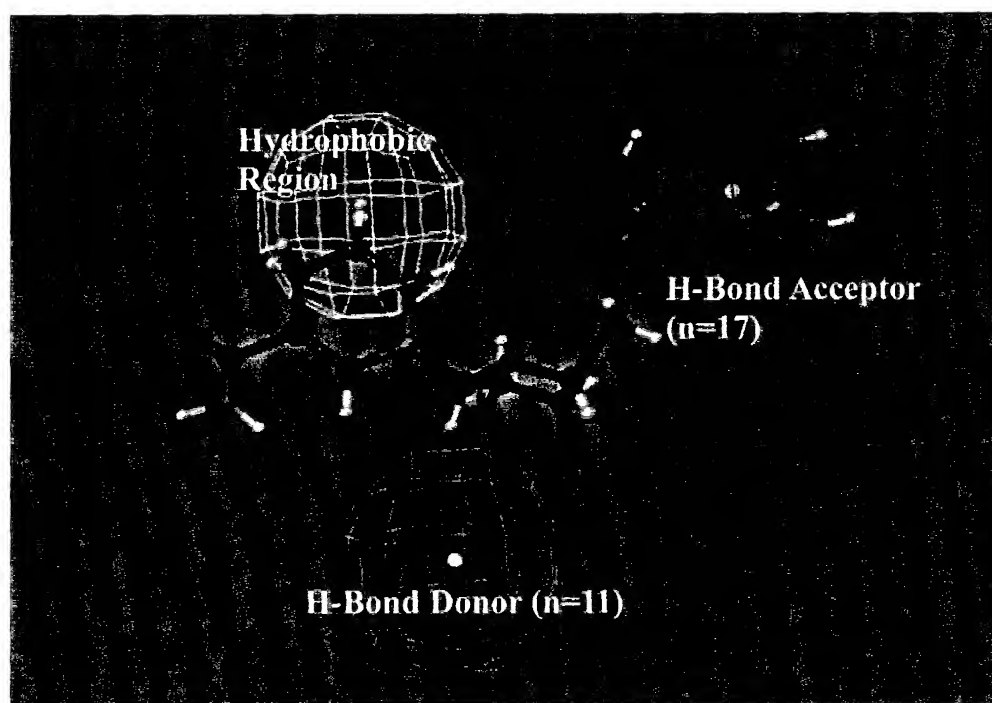
$K_{is} > 1 \text{ mM}$

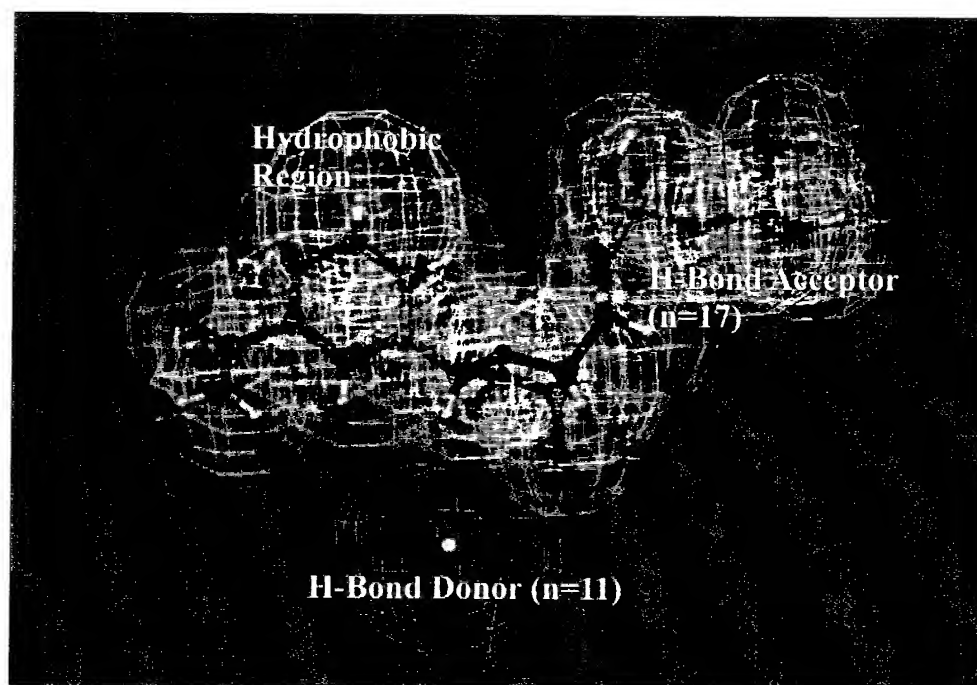
**A.**  
Compound: TTE0001.002.D2  
Pharmacofamily 1 exemplar



100409916 5680400T



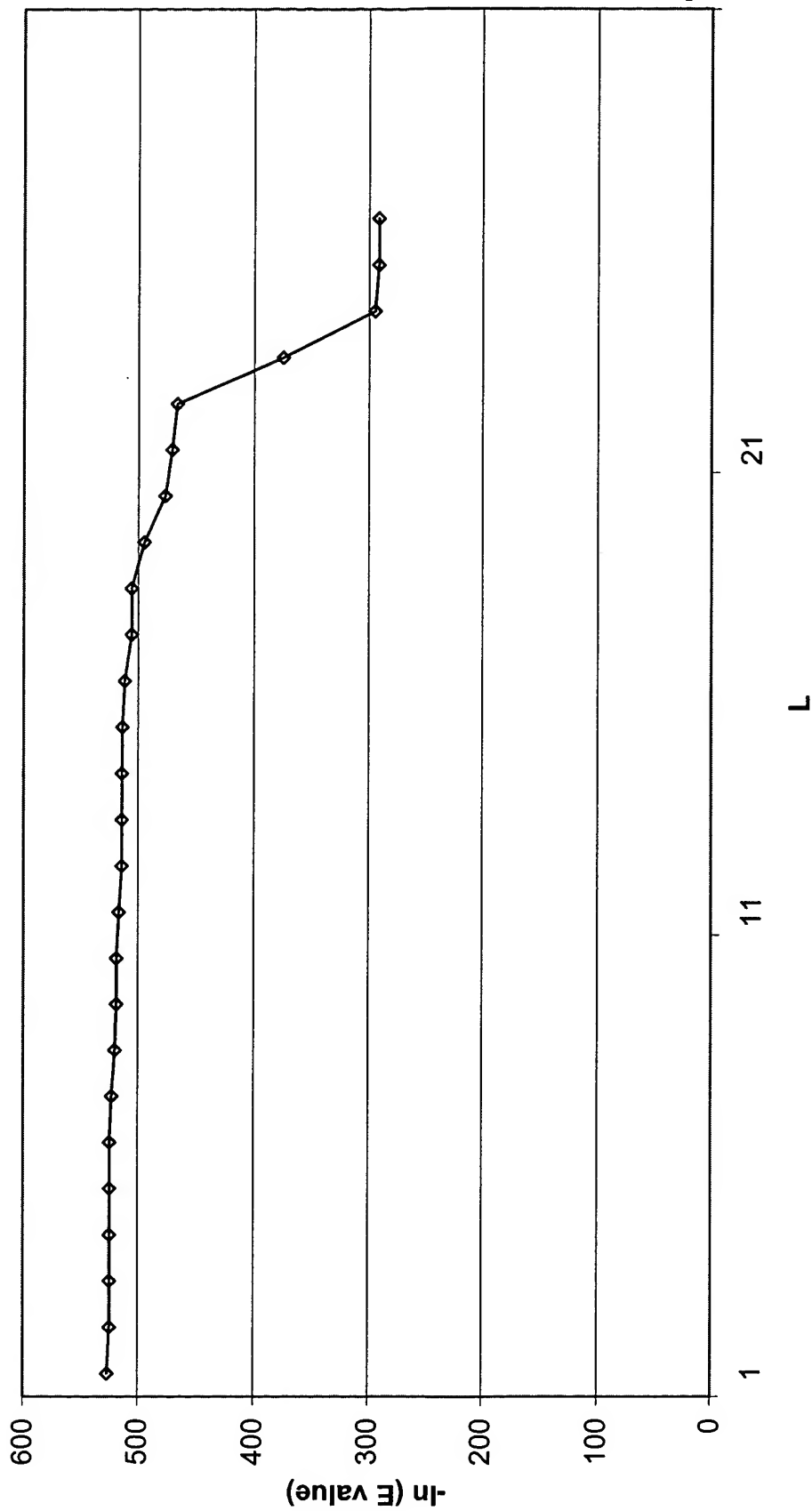




10040895 12301  
T04322 " 5680400T

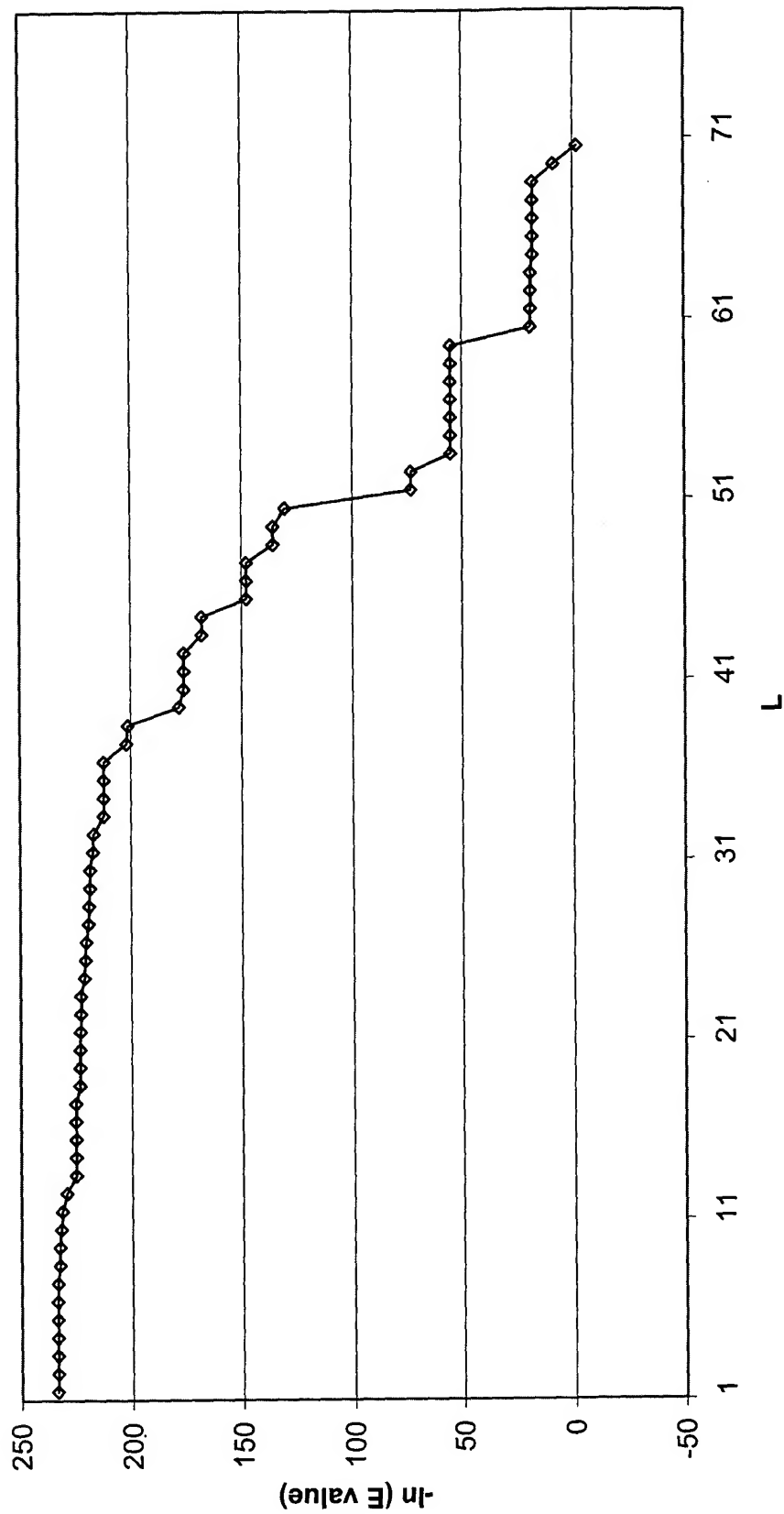


### Pharmacofamily 5



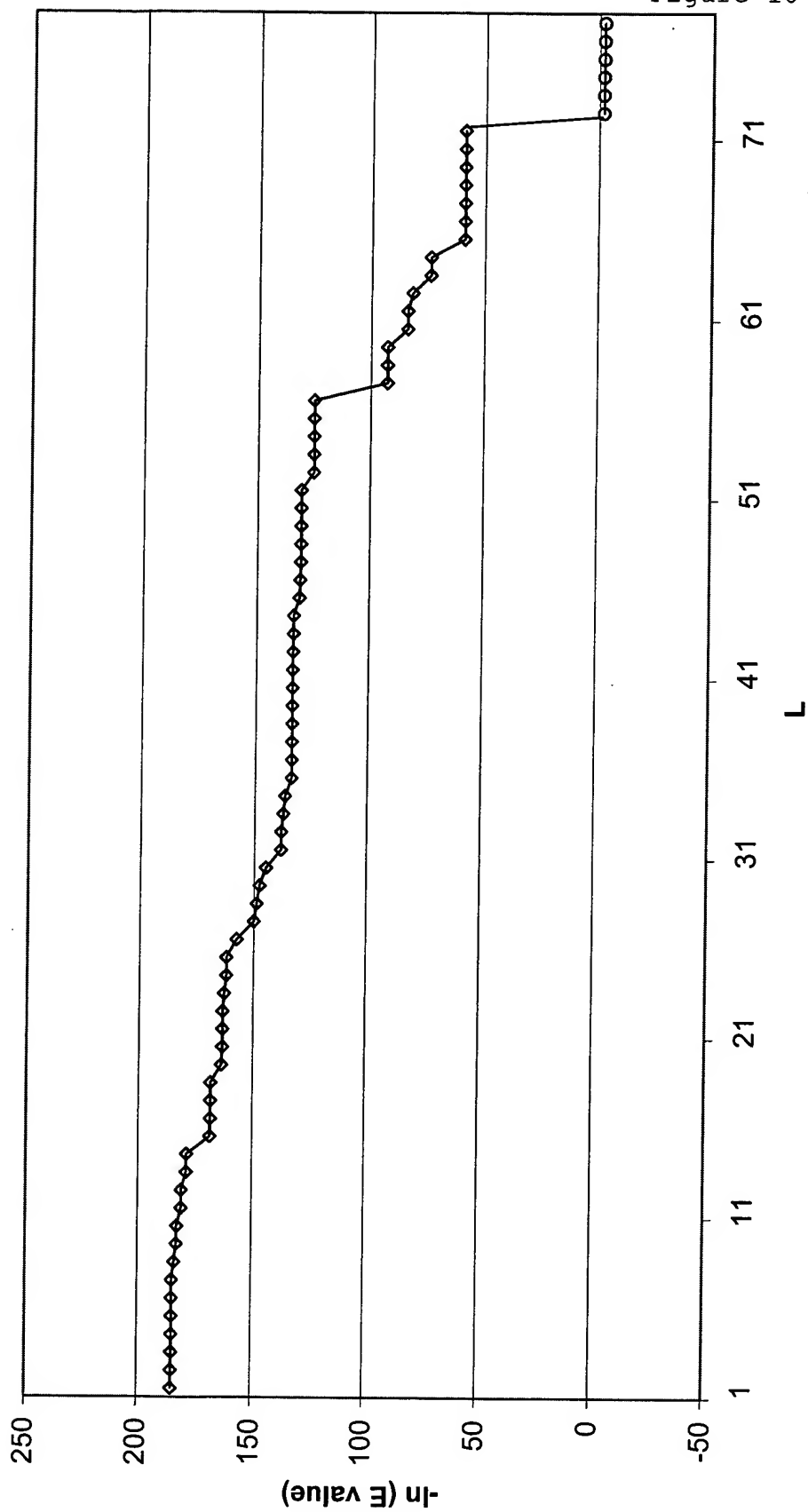
TEST "5650400T"

### Pharmacofamily 3 : Training Set 1



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Figure 9

# Pharmacofamily3 : Training Set 2



refinement cycle 5  
profile center:1AGN  
profile length: 599  
1AGN  
1AXE  
1YKF  
1HYH  
1LDN  
1EMD  
9LDB  
4MDH  
1BMD  
1PSD  
1DXY  
2NAD  
1A4I  
1B3R  
1PJC  
1ARZ  
1QR6

1AGN:	.....	.CL.....	.....	IGC.	.GFSTGYGAA	VKTGK...V.
1AXE:	.....	.....	.....	GC.	.GFSTGYGSA	VKVAK...V.
1YKF:	.....	.VM.....	.....	IPD.	.MMTTGFHGA	E.LAD...I.
1HYH:	.....	.....	.....	.....	.....	.....
1LDN:	.....	.....	.....	.....	.....	.....
1EMD:	.....	.....	.....	.....	.....	.....
9LDB:	.....	.....	.....	.....	.ATLKDQL.	I.HNL...L.
4MDH:	.....	.....	.....	.....	.....	.....
1BMD:	.....	.....	.....	.....	.....	.....
1PSD:	.....P.....	.F.....	.....	SN.	.TRSV AELV.	IGELL.LLLR
1DXY:	...SNV...	.P.....	.....	AYS.	.PAAIAEFA.	LTDTL.YLLR
2NAD:	.....	.....	.....	CN.	.SISVAEHV.	VMMIL.SLVR
1A4I:	.....	.....	.....	.....	.PCTPKGC.	LELIK.ET.G
1B3R:	.....	.....	.....	KFD.	.NLYGCRESL.	IDGIKRAT.D
1PJC:	.....	.....	.....	TPM	.SI.IAGRLSV	Q.FGA.RFLE
1ARZ:	.....	.....	.....	.....	.....	.....
1QR6:	LIQFEDFGNH	NAFRFLRK <del>Y</del> R	EKYCTFNDD.	.....	.IQGTAAVA.	LAGLL.AAQK

1AGN:	.....	.....	.....	.....	KP.....	.G.STCVVF.
1AXE:	.....	.....	.....	.....	TQ.....	.G.STCAVF.
1YKF:	.....	.....	.....	.....	EL.....	.G.ATVAVL.
1HYH:	.....	.....	.....	.....	.....	.A.RKIGIIG
1LDN:	.....	.....	.....	.....	.MK..NN	GG.ARVVVIG
1EMD:	.....	.....	.....	.....	.....	...MKVAVLG
9LDB:	.....	.....	.....	.....	.KEE...HV	PH.NKITVVG
4MDH:	.....	.....	.....	.....	.SE.....	.P.IRVLVTG
1BMD:	.....	.....	.....	.....	.MKA.....	.P.VRVAVTG
1PSD:	.GVPEANAK	A..HRGV.W.	NKL..AA.G.	SFEAR.....	.....	.G.KKLGII.
1DXY:	.NMGKVQAQ	L..QAGDYEK	AGT..F..I.	GKELG.....	.....	.Q.QTVGVM.
2NAD:	.NYLPSHE.	WARK.GGWN.	.IADCVSHA.	Y.DLE.....	.....	.A.MHVGTV.
1A4I:	.....	.....	.....	.....	.VPIA.....	.G.RHAVVV.
1B3R:	.....	.....	.....	.....	.VMIA.....	.G.KVAVVA.
1PJC:	RQQ.....	.....	.....	GGR	GVLLGGVPGV	KP.GKVVIL.
1ARZ:	.....	.....	.....	.....	...N.....	...IRVAIAG
1QR6:	..V.....	.....	.....	I.	SKP.I.....	.SEHKILFL.

T0040899 " 568400T

1AGN: GLGG.VGLSV IMGCK..SA. ....G... .A.SRIIGID ..L.N.....  
1AXE: GLGG.VGLSV IMGCK..AA. ....G... .A.ARIIGVD ..I.N.....  
1YKF: GIGP.VGLMA VAGAK..LR. ....G... .A.GRIIAGV ....S.....  
1HYH: L.GN.VGAAV AHGLIAQGV. .A..... .D..DYVFID A.N.E.....  
1LDN: A.GF.VGASY VFALMNQGI. .A..... .D..EIVLID A.N.E.....  
1EMD: AAGG.IGQAL ALLLKTQLP. .S...G... .S..ELSLYD I.A.P.....  
9LDB: V.GA.VGMAC AISILMKEL. .A..... .D..EIALVD V.M.E.....  
4MDH: AAGQ.IAYSL LYSIG.NG.S VFGKDQP... .I..ILVLLD ITP.MM....  
1BMD: AAGQ.IGYSL LFRIA.AG.E MLGKDQP... .V..ILQLLE I.PQAM....  
1PSD: GYGH.IGTQL GILAE..SL. ....G... .M..YVYFYD I...E.....  
1DXY: GTGH.IGQVA IKLFPK..GF. ....G... .A..KVIAVD P...Y.....  
2NAD: AAGR.IGLAV LRRLA..PF. ....D... .V..HLHYTD ....R.....  
1A4I: GRSKIVGAPM HDLLL..WN. ....N... .A..TVTTCH S...K.....  
1B3R: GYGD.VGKGC AQALR..GF. ....G... .A..RVIITE I...D.....  
1PJC: GGGV.VGTEA AKMAV..GL. ....G... .A..QVQIFD I...N.....  
1ARZ: AGGR.MGRQL IQAAL.ALE. GV..... .Q..LGAAL EREG.SS....  
1QR6: GAGE.AALGI ANLI...VS. ..VENGLSEQ EAQKKIW.FD K...YGLLVK

1AGN: ...KD.KFEK AM.AVGA... ..T.E.C...I  
1AXE: ...KD.KFAK AK.EVGA... ..T.E.C...V  
1YKF: ...RPVCVDA AK.YYGA... ..T.D.I...V  
1HYH: ...A..KVK. .A.D.QID.. FQ.....DAM ANL.EAH.G. NI.V.I...N  
1LDN: ...S..KAI. .G.D.AMD.. FN.....HGK V.FAPKP.V. DI.W.H...G  
1EMD: ...V...TP. .G.V.AVD.. LS.....HI. .P.P.TA.V. KI.K.G...F  
9LDB: ...D..KLK. .G.E.MD.. LQ.....HGS L.F..LR.TP KI.V.S...G  
4MDH: ...G..VLD. .G.V.LME.. L.....QDC ..A..LPPLK DV.I.A...T  
1BMD: ...K..ALE. .G.V.VME.. LE.....DCA .....FPLLA GL.E.A...T  
1PSD: ...N..K... .L...P.... LG..... NA.T.Q...V  
1DXY: .....P... .M.K.GD... HP..... DF.D.Y...V  
2NAD: ...H..R... .L.P..ES.. VE.....K .....E..L. NL.T.W...H  
1A4I: .....  
1B3R: ...PI.NAL..Q.A.AM... EG..... .Y.E.V...T  
1PJC: ...VERL... .SYL..ETL. FG.....S .....RV.ELL...Y  
1ARZ: ...L...LG. .S.D.A... GELAGAGK.T .....GV.T.V...Q  
1QR6: GRKAK..... .I.D...SYQ EP..... .FTHSAPESI

1AGN: S...PKDSTK PI.S.EVLSE M.T..G.NNV GYTFEVIG.. ...H.....  
1AXE: N...PQDYKK PI.Q.EVLTE M.S..N.GGV DFSFEVIG.. ...R.....  
1YKF: N...YKDG..PI.E.SQIMN L.T..EGKGV DAIIIAGG.. ...N.....  
1HYH: ...D..... .W....A. .ALAD...A DVVISTLG.. ...NIKLQQ.  
1LDN: ...D..... .Y....D. .DCRD...A DLVVICAG.. ...AN..QKP  
1EMD: SGE.D..... .A.T.PAL.. .E.G...A DVVLISAG.. ...VR..RK.  
9LDB: K...D..... .Y..NVT.. .A.N...S RLVVITAG.. ...AR..QQE  
4MDH: D...K..... .EEI..AFK. .D.....L DVAILVGS.. ...MP..RR.  
1BMD: D.D.P..... .D.V..AFK. .D.....A DYALLVGA.. ...AP.RKA.  
1PSD: Q.H.L..... .S.D..LLN. .M.....S DVVSLHVPEN .PST.....  
1DXY: S...L..... .E.D..LFK. .Q.....S DVIDLHVPGI .EQN.....  
2NAD: AT..R..... .E.D..MYP. .V.....C DVVTLNCPLH .PET.....  
1A4I: TAH..L..... .D.E..EVN. .K.....G DILVVATG.. ...Q.....  
1B3R: T...M..... .D.E..ACK. .E.....G NIFVTTG.. ...C.....  
1PJC: SNSAE..... IE.T..AVA. .E.....A DLLIGAVLVP GRR.....  
1ARZ: S...S..... .LDAV.K. .D.D....F DVFIDFT... ..R.....  
1QR6: PDT.F..... ED.A...VN. ILK.....P STIIGVAGA. ...G.....

1004095 12231

1AGN: .....L...ETM .I.DALA.SC ....HMNYGT SVVVGV..P.  
1AXE: .....L...DTM .V.TALS.CC ....QEAYGV SVIVGV..P.  
1YKF: .....A...DIM .A.TAVK.IV ....KPGGT IANVNY..F.  
1HYH: .....FA...E LKFTSSMV.Q S...V.GTNLK .ESGFH..GV LVVISN.P..  
1LDN: GET.RLD..L VDKNIAIF.R S..I.VESVM .ASGFQ..GL FLVATN.P..  
1EMD: PGMDRSD..L FNVNAGIV.K N..L.VQOVA .KT.CP.KAC IGIITN.P..  
9LDB: G.ESRLN..L VQRNVNIF.K F..I.IPNIV .KY.SP.NCK LLVVSN.P..  
4MDH: DGMERKDL.L .KANVKIF.K C..Q.GAALD .KY.AKKSVM VIVVSN.P..  
1BMD: .GM..ERRDL LQVNGKIF.T E..Q.GRALA .EV.AKKDVK VLVVGN.P..  
1PSD: .....K..NM.M GAKE.ISLM. ....KP.GSL LINASR.GT.  
1DXY: .....T..HI..I NEAA.FNLM. ....KP.GAI VINTAR.PN.  
2NAD: .....E..HM.I NDET.LKLF. ....KR.GAY IVNTAR.GK.  
1A4I: .....P..EM.V ...K.GEWI. ....KP.GAI VIDCGI..N.  
1B3R: .....V...DII ...L.GRHFE .Q..MKDDAI VCNIGH.F..  
1PJC: .....P...I..L ...VPASLVE .Q..MRTGSV IVDVAV.DO.  
1ARZ: .....P..EGTL N..H.LAFCR .Q..HG..KG MVIGTT..G.  
1QR6: .....R...L.F TPDV.IR..A AS..INERPV IFALSNPTAQ

1AGN: .PSA.K.M.. .L.TY.D.PM .....L...L... .....FT..  
1AXE: .PDS.Q.N.. .L.SM.N.PM .....L...L... .....LS..  
1YKF: .GE..GEV.. .L...PV .....PRL EWGC..G... .....MA..  
1HYH: .....V.D.. .V.I..TALF .....QHV.. .....TG..  
1LDN: .....V.D.. .I.L..TYAT .....WKF.. .....SG..  
1EMD: .....V.N.. .T.T..VAIA .....AEV.. .....LKKA  
9LDB: .....V.D.. .I.L..TYVA .....WKI.. .....SG..  
4MDH: .....A.N.. .T.N..CLTA .....SKS.. .....AP..  
1BMD: .....A.N.. .T.N..ALIA .....YKN.. .....AP..  
1PSD: .V...V.D.. .I.PA.LCDA .....L...A... .....SK..  
1DXY: .L...I.D.. .T.QA.MLSN .....L...K... .....SG..  
2NAD: .L...C.D.. .R.DA.VARA .....L...E... .....SG..  
1A4I: ..YKVV.G.. .D.VA.YD.E .....A... .K...E... .....  
1B3R: .....D.V.. .E.ID.VKW. ....LNEN. ...AVEKVNI KPQVDRL..  
1PJC: .....G.. .GCVETLHPT SHTQPTY... .E...V... .....  
1ARZ: .....F.DEA GK.QA.IRDA .....A..... .....AD..  
1QR6: AE...C.... .TAEE.AYTL .....T... .....E...

1AGN: .....GR.T WK.....GC .....  
1AXE: .....GR.T WK.....GA .....  
1YKF: .....HK.T IK.....GG .....  
1HYH: .....FPAHK VI..G...TG ....T.....  
1LDN: .....LPHER VI..G...S.....  
1EMD: GV...YDKNK LF..G...VT .....TL DI...IRSNT FVAEL..KGK  
9LDB: .....FPKNR VI..G...SG ....C...N.....  
4MDH: .S...IPKEN FS..C...LT .....RL DH...NRAKA QIALK..LGV  
1BMD: .G...LNPRN FT..A...MT .....R.....  
1PSD: .....H.LAG AA.....ID VFPTE...P..ATNSD....PF.T..S..  
1DXY: .....K.LAG VG.....ID TYEYETEDL..LN..LAKH. GSFKDPLW.D  
2NAD: .....R.LAG YA.....GD VWFPQ...P..A.....PK.D..H..  
1A4I: .....R.ASF IT..PVPGGV ....G...P.....  
1B3R: .LKNGHRI.I LLAEG...RL V...N...L.....  
1PJC: .....FGV.V HY..G...VP .....  
1ARZ: .....I.A IV..F...A.A..N.....  
1QR6: .....GRC LF..A...SG SP..F.....G.P

10040305.1.2201



```

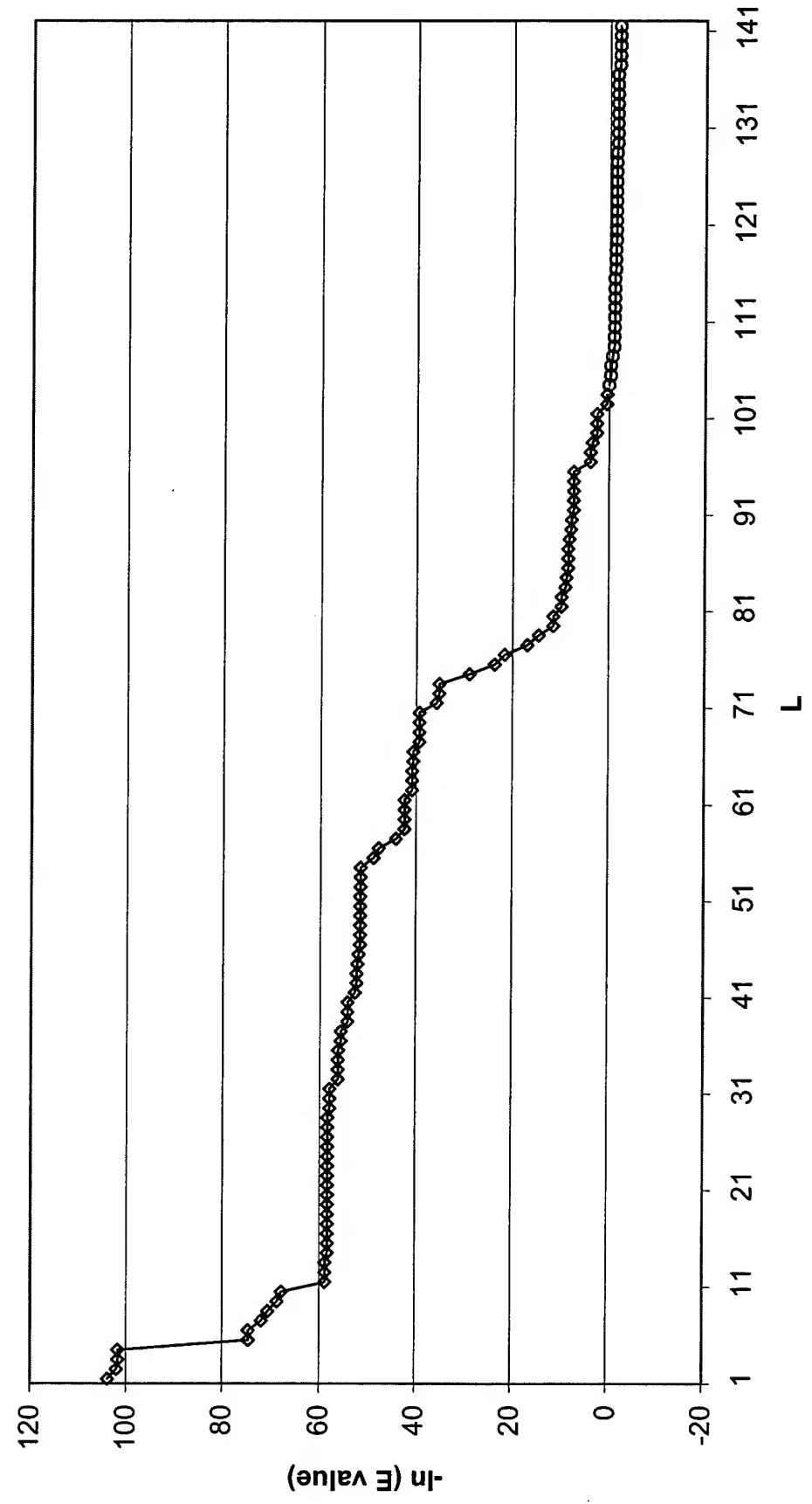
1AGN: .....
1AXE: .....
1YKF: .....
1HYH: .....
1LDN: .....
1EMD: K.S....I.G TLSAFEQNAL EG.ML...DT LKK.DIALGQ EF..VNK..
9LDB: .....
4MDH: I.V....EGL PI.N..DFS. REKMDLTAK L.AEE..KET AFEFL.SSA
1BMD: .....
1PSD: .....
1DXY: .....
2NAD: .....
1A4I: .....
1B3R: .....
1PJC: .....
1ARZ: ...VLDLN.N L.....
1QR6: QGRLYPPL.A NIQE.VSINI AIKVTEYLYA NKAFRYPEPE DKAKYVKER

```

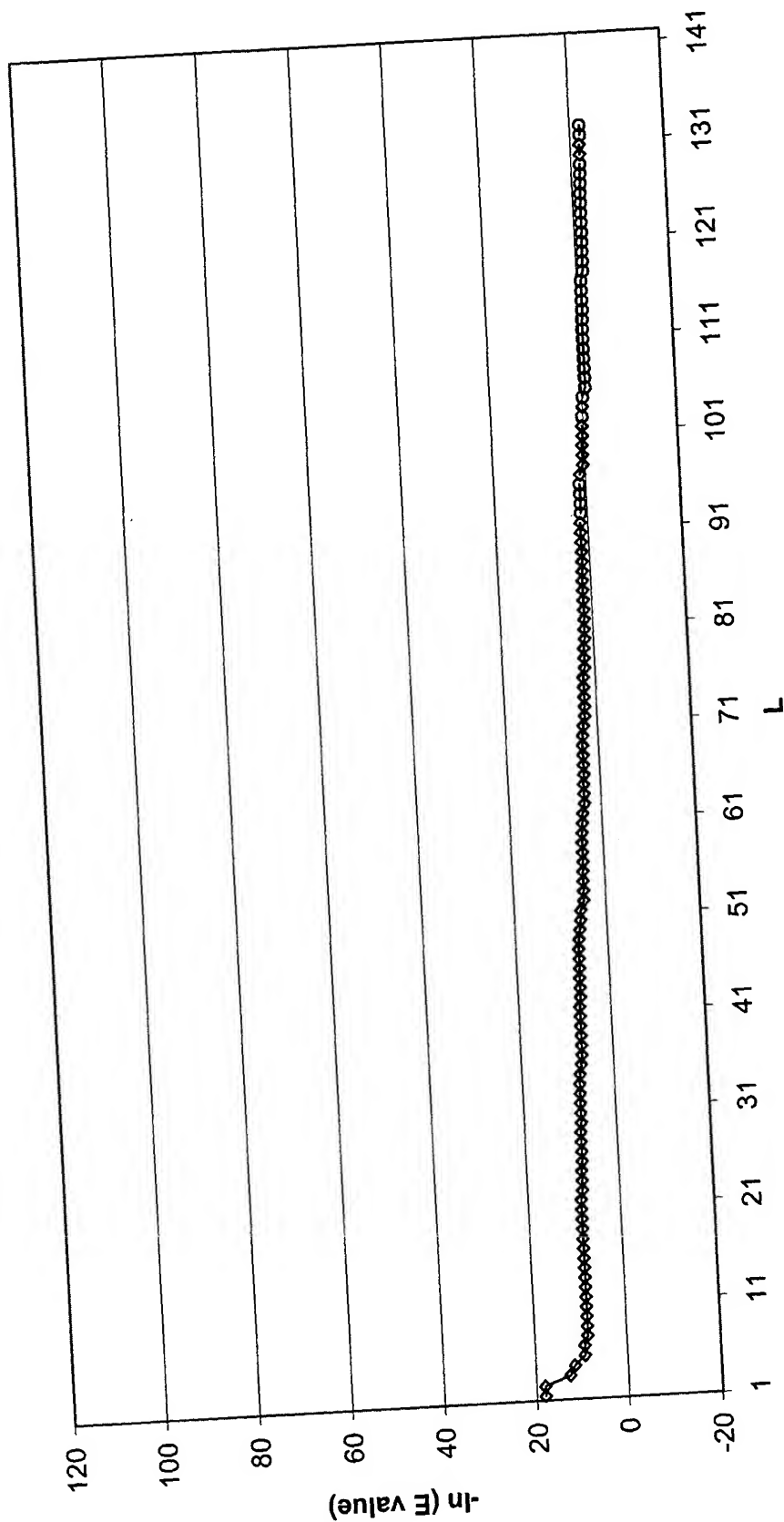


TC822T"5680400T

# Pharmacofamily 1

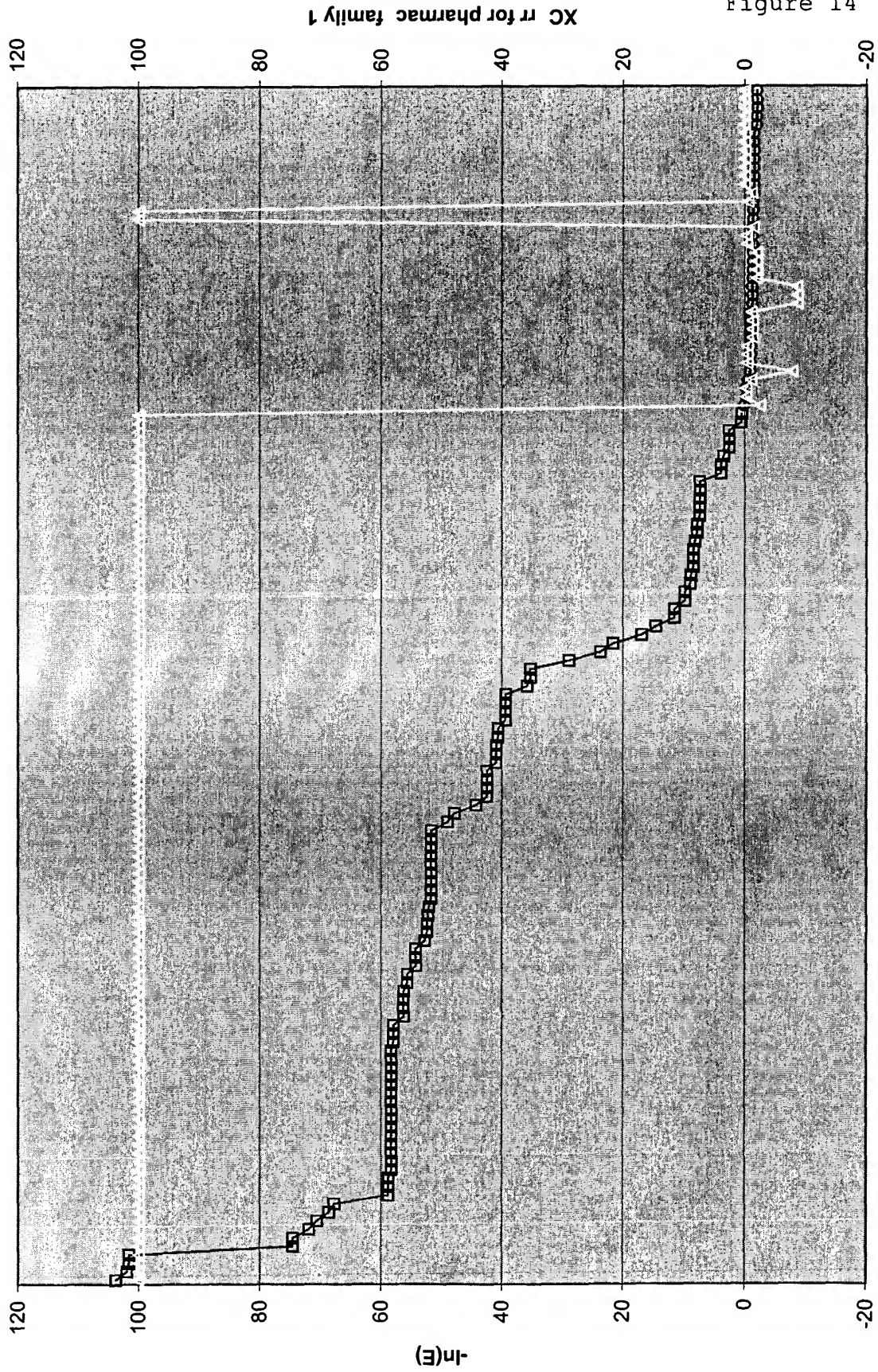


# Pharmacofamily 1 with Differential Filtering



T0822T-5698400T

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Figure 14



PDB Proteins for Pharmacofamily 1